

Benzonitrile
100-47-0 | DTXSID7021491

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 6.39 days

Global applicability domain: Outside

Local applicability domain index: 3.69e-01

Confidence level: 7.17e-01

Nearest Neighbors from the Training Set

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Ethylcyclopentane

Measured: 511

Predicted: 8.14

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Ethylcyclohexane

Measured: 4.93

Predicted: 3.02

[Image not found](#)

Pentane

Measured: 40.7

Predicted: 6.52

[Image not found](#)

n-Hexane

Measured: 157

Predicted: 7.45

[Image not found](#)

Ethylbenzene

Measured: 120

Predicted: 6.21